

VNMR 3D processing of States-TPPI (t1) PFG (t2) data sets.

Processing procedure

This procedure applies to data acquired using States-TPPI during t_1 and PFG during t_2 . The procedure is similar to 2D data processing when processing the f_{3f2} and f_{3f1} planes. Remember to adjust the window function, linear predictions parameters, and zero filling as required.

1. Process 2

A. for **array = 'phase,phase2'**

```
wft2d('ni2',1, 1,0,1,0, 0,0,0,0, 0,-1,0,1, 0,0,0,0)
```

If by some reason the f_1 axis is inverted use,

```
wft2d('ni2',1, 1,0,1,0, 0,0,0,0, 0,1,0,-1, 0,0,0,0)
```

B. for **array = 'phase2,phase'**

```
wft2d('ni2',1, 1,0,0,0, 1,0,0,0, 0,-1,0,0, 0,1,0,0)
```

Again if by some reason the f_1 axis is inverted use,

```
wft2d('ni2',1, 1,0,0,0, 1,0,0,0, 0,1,0,0, 0,-1,0,0)
```

2. Process 1

A. for **array = 'phase,phase2'**

```
wft2d('ni',1, 1,0,1,0, 0,0,0,0, 0,0,0,0, 1,0,1,0)
```

If by some reason the f_1 axis is inverted use,

```
wft2d('ni',1, 1,0,1,0, 0,0,0,0, 0,0,0,0, -1,0,-1,0)
```

B. for **array = 'phase2,phase'**

```
wft2d('ni',1, 1,0,0,0, 1,0,0,0, 0,0,1,0, 0,0,1,0)
```

Again if by some reason the f_1 axis is inverted use,

```
wft2d('ni',1, 1,0,0,0, 1,0,0,0, 0,0,-1,0, 0,0,-1,0)
```

3. Coefficients are now stored in `~/vnmrsys/coeflib`. The proper coefficients can be set by invoking the **coef** macro in `vnmr`. This will determine the proper coefficients to be used in your 3D experiments. This macro will only work with the variables `phase` and `phase2` for quadrature detection and gradient sign selection.

4. The coefficients can be obtained by substituting in the following table:

array = phase2,phase

ni	1a	2a	3a	4a		0	0	0	0		5a	6a	7a	8a		0	0	0
ni2	1b	2b	0	0		3b	4b	0	0		5b	6b	0	0		7b	8b	0

1b	2b	0	0		3b	4b	0	0
0	0	-1b	-2b		0	0	-3b	-4b
-5b	-6b	0	0		-7b	-8b	0	0
0	0	5b	6b		0	0	7b	8b
1a	2a	3a	4a		5a	6a	7a	8a

array = phase,phase2

ni	1a	2a	0	0		3a	4a	0	0		5a	6a	0	0		7a	8a	0
ni2	1b	2b	3b	4b		0	0	0	0		5b	6b	7b	8b		0	0	0

1b	2b	3b	4b		0	0	0	0
0	0	0	0		-1b	-2b	-3b	-4b
-5b	-6b	-7b	-8b		0	0	0	0
0	0	0	0		5b	6b	7b	8b
1a	2a	3a	4a		5a	6a	7a	8a

Example:

If you collected the data using **array = 'phase,phase2'** used the following to obtain the 1 3

and 2 3

wft2d('ni',1, 1,0,1,0, 0,0,0,0, 0,0,0,0, 1,0,1,0)

wft2d('ni2',1, **1,0,1,0, 0,0,0,0, 0,-1,0,1, 0,0,0,0**)

where the coefficients are

ni	1a	2a	0	0		3a	4a	0	0		5a	6a	0	0		7a	8a	0
	1	0	1	0		0	0	0	0		0	0	0	0		1	0	1
ni2	1b	2b	3b	4b		0	0	0	0		5b	6b	7b	8b		0	0	0
	1	0	1	0		0	0	0	0		0	-1	0	1		0	0	0

then the 3D coefficients will be

1b	2b	3b	4b		0	0	0	0
1	0	1	0		0	0	0	0
0	0	0	0		-1b	-2b	-3b	-4b
0	0	0	0		-1	0	-1	0
-5b	-6b	-7b	-8b		0	0	0	0
0	1	0	-1		0	0	0	0
0	0	0	0		5b	6b	7b	8b
0	0	0	0		0	-1	0	1
1a	2a	3a	4a		5a	6a	7a	8a
1	0	0	0		0	0	1	0

```

1 0 1 0 0 0 0 0
0 0 0 0 0 -1 0 -1
0 1 0 -1 0 0 0 0
0 0 0 0 0 -1 0 1
1 0 0 0 0 0 1 0
    
```